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Standard Reference Data Publications 1987-1989

Joan C. Sauerwein

Standard Reference Data
National Institute of Standards and Technology
Gaithersburg, MD 20899

December 1989



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Foreword

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The Standard Reference Data Program of the National Institute of Standards and Technology coordinates this effort which involves many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated physical and chemical property data. These compilations are published in the Journal of Physical and Chemical Reference Data and through other appropriate channels. Other outputs of the program include bibliographies, computer programs for handling data, and databases in magnetic tape and disk formats.

This listing includes all publications which have appeared in the period 1987–1989. It supplements “Standard Reference Data Publications 1964–1984” (SP708) and “Standard Reference Data Publications 1985–1986” (SP708, Supplement 1). Indexes to authors, properties, and material classes are given, as well as information on ordering publications.

Malcolm W. Chase, Jr.
Acting Chief
Standard Reference Data

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Standard Reference Data Publications 1987-1989

Joan C. Sauerwein

Standard Reference Data, National Institute of Standards and Technology, Gaithersburg, MD 20899

The National Institute of Standards and Technology's Standard Reference Data Program manages a network of data centers that prepare evaluated databases of physical and chemical properties of substances. Databases are available in printed form, on magnetic tapes, diskettes, and through on-line computer networks. This document provides a comprehensive list of the products available from the National Standard Reference Data System (NSRDS) for the years 1987-1989, including indexes qualified by author, material, and property terms. Ordering information and current prices can be found at the end of this document.

Key words: bibliographies; chemical properties; evaluated data; indexes; materials properties; physical properties; publication list.

Introduction

The National Standard Reference Data System (NSRDS), established in 1963, coordinates on a national scale the compilation and dissemination of reference data in the physical sciences. Under the Standard Reference Data Act (Public Law 90-396) the National Institute of Standards and Technology (NIST) of the U.S. Department of Commerce has the primary responsibility in the Federal Government for providing reliable scientific and technical data. Standard Reference Data at NIST coordinates a complex of data evaluation centers, located in university, industrial, and other Government laboratories as well as within NIST. These centers compile and critically evaluate numerical physical and chemical property data retrieved from the world's scientific literature.

This publications list includes NSRDS data compilations, critical reviews, and other publications which are available from various sources. Indexes by author, property, and materials class are included. Prices and ordering instructions for publications listed are given in this document and further information may be obtained from:

Standard Reference Data
National Institute of Standards and Technology
Gaithersburg, MD 20899
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My thanks to Gerry Dalton, Mary Trapani and Linda Bastiani for their help in the preparation of this document.

Reprints

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Thermochemical Data on Gas Phase Compounds of Sulfur, Fluorine, Oxygen, and Hydrogen Related to Pyrolysis and Oxidation of Sulfur Hexafluoride - John T. Herron. *J. Phys. Chem. Ref. Data* 16, 1 (1987).

Thermochemical data on selected gas phase compounds containing sulfur, fluorine, oxygen, and hydrogen are evaluated. These are of particular relevance to plasma chemistry and SF₆ dielectric breakdown. Values of the enthalpies of formation and the entropy are provided at 298 K. Where no experimental data are available, methods for estimation have been developed for deriving the enthalpy of formation. Data are tabulated for 36 substances.

311

The Thermochemical Measurements on Rubidium Compounds: A Comparison of Measured Values with Those Predicted from the NBS Tables of Chemical and Thermodynamic Properties - V. B. Parker, W. H. Evans and R. L. Nuttall. *J. Phys. Chem. Ref. Data* 16, 7 (1987).

This report presents the assessed thermochemical measurements on rubidium compounds upon which the property values, $\Delta_f H^\circ$, $\Delta_f G^\circ$, S° , C_p° , and $H^\circ(T) - H^\circ(0)$ at 298.15 K and $\Delta_f H^\circ(0 \text{ K})$ recommended in the "NBS Tables of Chemical Thermodynamic Properties" are based. Included in this set of thermochemical measurements, or thermochemical reaction catalog, is a comparison of the observed values for the processes in question with those predicted (calculated) from the recommended property values in the forementioned tables.

312

Standard Thermodynamic Functions of Gaseous Polyatomic Ions at 100-1000 K - Aharon Loewenschuss and Yitzhak Marcus. *J. Phys. Chem. Ref. Data* 16, 61 (1987).

The standard thermodynamic functions—heat capacity at constant pressure C_p° , its ratio to that at constant volume, the entropy S° , the enthalpy minus that at absolute zero ($H^\circ - H^\circ_0$), and the Gibbs energy function ($G^\circ - H^\circ_0$)/ T were calculated for 131 gaseous ions in the temperature interval 100-1000 K, and are presented in tables. The input data included structural information (bond lengths and angles), vibrational spectroscopic information (vibrational frequencies and degeneracies), and electronic level occupation and degeneracies for ions having unpaired electrons.

313

Thermodynamic Properties of Manganese and Molybdenum - P. D. Desai. *J. Phys. Chem. Ref. Data* 16, 91 (1987).

This work reviews and discusses the data on the various thermodynamic properties of manganese and molybdenum available through March 1985. These include heat capacity, enthalpy, enthalpy of transitions and melting, vapor pressure, and enthalpy of vaporization. The existing data have been critically evaluated and analyzed. The recommended values for the heat capacity, enthalpy, entropy, and Gibbs energy function from 0.5 to 2400 K for manganese and from 0.4 to 5000 K for molybdenum have been generated, as have heat capacity values for supercooled β -Mn and for γ -Mn below 298.15 K. The recommended values for vapor pressure cover the temperature range from 298.15 K to 2400 K for manganese and from 298.15 K to 5000 K for molybdenum. These values are referred to temperatures based on IPTS-1968. The uncertainties in the recommended values of the heat capacity range from $\pm 3\%$ to $\pm 5\%$ for manganese and from $\pm 1.5\%$ to $\pm 3\%$ for molybdenum.

314

Thermodynamic Properties of Selected Binary Aluminum Alloy Systems - P. D. Desai. *J. Phys. Chem. Ref. Data* 16, 109 (1987).

This work reviews the data and information available through March 1985 on the various thermodynamic properties of five binary

aluminum alloy systems: Al-Fe, Al-Mn, Al-Ni, Al-Si, and Al-Ti. The thermodynamic properties covered in this work are heat capacity, Gibbs energy, enthalpy, and entropy of formation. Existing data have been evaluated and analyzed. The values for heat capacity and room-temperature enthalpy of formation for a large number of alloys have been generated. For each of the binary alloy systems, the recommended values for integral Gibbs energy, enthalpy, and entropy of formation as well as the partial quantities, activity, and activity coefficients for each component covering the entire composition range have been reported. These values are reported for both solid and liquid alloys.

315

¹³C Chemical Shieldings in Solids - T. M. Duncan. *J. Phys. Chem. Ref. Data* 16, 125 (1987).

Analogous to the importance of ¹³C isotropic shieldings for chemical analysis of liquids with nuclear magnetic resonance spectroscopy, ¹³C chemical shielding anisotropies are proving to be valuable in the characterization of solids. Specifically, molecular geometry is revealed by the full shielding anisotropy and molecular motion may be characterized by changes in the powder pattern. In particular, the principal components of the shielding reveal differences in bonding geometry which may not be correlated to monotonic changes in the isotropic shift. This report is a comprehensive, critical compilation of ¹³C chemical shieldings in solids, organized by carbon functionality. From these data, representative shieldings of common carbon functionalities are calculated.

316

The Mark-Houwink-Sakurada Relation for Poly(Methyl Methacrylate) - Herman L. Wagner. *J. Phys. Chem. Ref. Data* 16, 165 (1987).

In this third review of a series, the literature values for the viscosity-molecular weight relationship (Mark-Houwink-Sakurada) for poly(methyl methacrylate) have been critically evaluated. Although most of the studies have been concerned with conventionally produced poly(methyl methacrylate), some work has also been done with the isotactic polymer. The Mark-Houwink relations for the following solvents are discussed: benzene, toluene, acetone, chloroform, 2-butanone, and tetrahydrofuran, as well as for several other infrequently used solvents.

The values of the coefficient K in the relation $[\eta] = KM^{0.5}$ for several theta solvents are also reported.

317

The Viscosity of Carbon Dioxide, Methane, and Sulfur Hexafluoride in the Limit of Zero Density - R. D. Trengove and W. A. Wakeham. *J. Phys. Chem. Ref. Data* 16, 187 (1987).

This paper contains accurate representations for the viscosity of the three polyatomic gases, carbon dioxide, methane, and sulfur hexafluoride, in the limit of zero density. These gases were studied because they possess permanent multipole moments of increasing order 4, 6, and 8, respectively. The correlations have associated uncertainties of $\pm 0.3\%$ around room temperature rising to $\pm 1.5\%$ at the low-temperature extreme and to a maximum of $\pm 2.0\%$ at the high-temperature extreme. The correlating equation for carbon dioxide is valid for the temperature range 200-1500 K, that for methane from 110-1050 K and that for sulfur hexafluoride from 220-900 K. It is shown that a two-parameter law of corresponding states is inadequate for the representation of the data over these wide ranges of temperature.

318

The Viscosity of Normal Deuterium in the Limit of Zero Density - M. J. Assael, S. Mixafendi and W. A. Wakeham. *J. Phys. Chem. Ref. Data* 16, 189 (1987).

This paper contains a new representation of the viscosity of normal deuterium in the limit of zero density as a function of temperature. The correlation is based upon the semiclassical kinetic theory of polyatomic gases and a body of critically evaluated experimental data. The similar-

ity of the intermolecular pair potentials of normal hydrogen and normal deuterium is employed to extrapolate the correlation for deuterium beyond the range of the experimental data. In the temperature range 250-350 K the accuracy of the representation of the viscosity is estimated to be $\pm 1\%$, which deteriorates to $\pm 2\%$ at the lowest temperatures and to $\pm 4\%$ at the highest temperatures.

319

Standard Chemical Thermodynamic Properties of Alkanethiol Isomer Groups - Robert A. Alberty, Ellen Burmenko, Tae H. Kang, and Michael B. Chung. *J. Phys. Chem. Ref. Data* 16, 193 (1987).

The chemical thermodynamic properties of alkanethiol (RSH where R is an alkyl group) isomer groups from CH_3S to $\text{C}_4\text{H}_{10}\text{S}$ in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of $\text{C}_5\text{H}_{12}\text{S}$ to $\text{C}_8\text{H}_{18}\text{S}$ have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K. For isomer group properties, increments per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Values of C_p° , S° , $\Delta_f H^\circ$, and $\Delta_f G^\circ$ are given for all species of alkanethiols from CH_3S to $\text{C}_8\text{H}_{18}\text{S}$ in SI units for a standard state pressure of 1 bar.

320

Evaluation of Binary Excess Volume Data for the Methanol + Hydrocarbon Systems - R. Srivastava and B. D. Smith. *J. Phys. Chem. Ref. Data* 16, 209 (1987).

The volume change of mixing data for the methanol + hydrocarbon binary mixtures have been compiled and the best sets of data identified. The needs for new experimental data have been defined.

321

Evaluation of Binary Excess Enthalpy Data for the Methanol + Hydrocarbon Systems - R. Srivastava and B. D. Smith. *J. Phys. Chem. Ref. Data* 16, 219 (1987).

The heat of mixing data for the methanol + hydrocarbon binary mixtures have been compiled and the best sets of data identified. The needs for new experimental data have been defined.

322

Extinction Coefficients of Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases: A Least-Squares Analysis - Ian Carmichael, W. P. Helman, and G. L. Hug. *J. Phys. Chem. Ref. Data* 16, 239 (1987).

A global least-squares technique is developed to assist in the critical evaluation of data consisting of large sets of measurements. The technique is particularly designed to handle sets of data where many of the measurements are relative measurements. A linearization procedure is used to reduce the inherently nonlinear problem to a traditional multivariate linear regression. The technique developed here is used to evaluate extinction coefficients, ϵ° , of triplet-triplet absorption (TTA) spectra of organic molecules in condensed phases.

323

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen (O^3P) with Unsaturated Hydrocarbons - R. J. Cvetanovic. *J. Phys. Chem. Ref. Data* 16, 261 (1987).

Chemical kinetic data for reactions of O^3P atoms with unsaturated hydrocarbons are compiled and critically evaluated. Specifically, the reactions considered include the interactions of the ground electronic state of oxygen atoms, O^3P , with alkenes, cycloalkenes, halogen substituted alkenes and ketenes, alkynes, halogen substituted alkynes, aromatic hydrocarbons and pyridine. All kinetic data considered were restricted to gas phase reactions. "Recommended" values of the rate parameters have been assessed and conservative uncertainty limits assigned to them.

324

Spectral Data for Molybdenum Ions, Mo VI - Mo XLII - Toshizo Shirai, Yohta Nakai, Kunio Ozawa, Keishi Ishii, Jack Sugar and Kazuo Mori. *J. Phys. Chem. Ref. Data* 16, 327 (1987).

Wavelengths, intensities, and classifications for the molybdenum ions Mo VI - Mo XLII are compiled. A short review of the work on each stage of ionization is included. The data are critically evaluated and the best results are quoted.

325

Standard Chemical Thermodynamic Properties of Alkanol Isomer Groups - Robert A. Alberty, Michael B. Chung, and Theresa M. Flood. *J. Phys. Chem. Ref. Data* 16, 391 (1987).

The chemical thermodynamic properties of alkanol (ROH) isomer groups from CH_3O to $\text{C}_4\text{H}_{10}\text{O}$ in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of $\text{C}_5\text{H}_{12}\text{O}$ to $\text{C}_8\text{H}_{18}\text{O}$ have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000 K.

326

High-Temperature Vaporization Behavior of Oxides II. Oxides of Be, Mg, Ca, Sr, Ba, B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, Zn, Cd, and Hg - R. H. Lamoreaux, D. L. Hildenbrand and L. Brewer. *J. Phys. Chem. Ref. Data* 16, 419 (1987).

In order to assess the high-temperature vaporization behavior and equilibrium gas phase compositions over the condensed oxides of Be, Mg, Ca, Sr, Ba, B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, Zn, Cd, and Hg, the relevant thermodynamic and molecular constant data have been compiled and critically evaluated. Selected values of the Gibbs energy functions of condensed and vapor phases are given in the form of equations valid over wide temperature ranges, along with the standard entropies and enthalpies of formation.

327

Equilibrium and Transport Properties of Eleven Polyatomic Gases at Low Density - A. Boushehri, J. Bzowski, J. Kestin, and E. A. Mason. *J. Phys. Chem. Ref. Data* 16, 445 (1987).

This study presents a computer programmable, thermodynamically consistent representation of the second virial coefficient B, viscosity η , self-diffusion coefficient D, and isotopic thermal diffusion factor α_0 of the eleven gases: N_2 , O_2 , NO, CO, N_2O , CO_2 , CH_4 , CF_4 , SF_6 , C_2H_4 , and C_2H_6 , all at low density. Limited thermodynamic consistency is achieved by the use of four scaling parameters (σ , ϵ , V^* , ρ^*) in addition to the molecular weight.

328

The Thermochemistry of Inorganic Solids IV. Enthalpies of Formation of Compounds of the Formula MX_aY_b - Mohamed W. M. Hisham and Sidney W. Benson. *J. Phys. Chem. Ref. Data* 16, 467 (1987).

It is found that the standard enthalpies of formation $\Delta_f H^\circ_{298}$ of double salts of the type MX_aY_b are related by a simple additivity relation to $\Delta_f H^\circ_{298}$ of their binary salts MX_a and MY_b .

329

Chemical Kinetic Data Base for Combustion Chemistry. Part 2. Methanol - Wing Tsang. *J. Phys. Chem. Ref. Data* 16, 471 (1987).

This publication contains evaluated and estimated data on the kinetics of reactions involving methanol and hydroxymethyl radicals and various small inorganic and organic species which are of importance for the proper understanding of methanol combustion and pyrolysis.

Phase Diagrams and Thermodynamic Properties of the 70 Binary Alkali Halide Systems Having Common Ions - James Sangster and Arthur D. Pelton. *J. Phys. Chem. Ref. Data* 16, 509 (1987).

A very extensive literature survey of all available phase diagrams and thermodynamic data has been carried out for all 40 possible common-anion binary systems (AX-BX) and all 30 possible common-cation binary systems (AX-AY) involving the alkali halides (A,B = Li, Na, K, Rb, Cs; X, Y = F, Cl, Br, I). A critical analysis and evaluation of these data have been performed with a view to obtaining a "best" evaluated phase diagram and a set of "best" evaluated thermodynamic parameters for each system.

331

Thermophysical Properties of Fluids. II. Methane, Ethane, Propane, Isobutane, and Normal Butane - B. A. Younglove and J. F. Ely. *J. Phys. Chem. Ref. Data* 16, 577 (1987).

Tables of methane, ethane, propane, isobutane and normal butane thermodynamic and transport properties are presented. The mathematical relations from which these thermophysical properties are obtained are described. The tables list pressure, density, temperature, internal energy, enthalpy, entropy, specific heat at constant pressure and at constant volume, sound speed, viscosity, thermal conductivity, and dielectric constant.

332

Methanol Thermodynamic Properties from 176 to 673 K at Pressures to 700 Bar - Robert D. Goodwin. *J. Phys. Chem. Ref. Data* 16, 799 (1987).

Available data for vapor pressures and for the orthobaric densities of methanol are examined and formulated. Then PpT data are correlated by an equation of state (EOS) which is constrained to the given coexistence boundary. Via ideal gas state specific heats, the thermodynamic properties of methanol then are obtained by numerical integrations of the EOS, and are tabulated along isobars. A comparison is made with some recent calorimetric enthalpy differences data over a wide range of the EOS surface.

333

International Equations for the Saturation Properties of Ordinary Water Substance - A. Saul and W. Wagner. *J. Phys. Chem. Ref. Data* 16, 893 (1987).

Consistent with the latest experimental data and the recent internationally recommended values for the critical parameters, we have developed compact and accurate representative equations for the following properties on the saturation line of ordinary (light) water substance: vapor pressure, density, enthalpy and entropy of both the saturated liquid and the saturated vapor.

334

Rate Data for Inelastic Collision Processes in the Diatomic Halogen Molecules. 1986 Supplement - J. I. Steinfeld. *J. Phys. Chem. Ref. Data* 16, 903 (1987).

The previously published compilation of rate data for inelastic collision processes involving the homonuclear and heteronuclear diatomic halogen molecules [*J. Phys. Chem. Ref. Data* 13, 445 (1984)] has been updated through June, 1986. Additional data on collision processes involving the interhalogens, and on processes at very low kinetic temperatures, are presented; in addition, several previously accepted rate data have been corrected.

335

Critical Survey of Data on the Spectroscopy and Kinetics of Ozone in the Mesosphere and Thermosphere - Jeffrey I. Steinfeld, Steven M. Adler-Golden, and Jean W. Gallagher. *J. Phys. Chem. Ref. Data* 16, 911 (1987).

Spectroscopic data and reaction rate coefficients pertinent to ozone in the mesosphere and thermosphere (altitude > 50 km) are critically surveyed. These data should be of use in modeling atmospheric infrared luminescence, measuring atmospheric ozone concentrations by remote sensing, and designing and interpreting laboratory measurements.

336

Critical Compilation of Surface Structures Determined by Low-Energy Electron Diffraction Crystallography - Philip R. Watson. *J. Phys. Chem. Ref. Data* 16, 953 (1987).

This review critically compiles all surface structures derived from low-energy electron diffraction (LEED) crystallography reported in the refereed literature prior to January 1986. Over 250 investigations have been analyzed covering all types of surfaces including clean and adsorbate-covered metal, semiconductor and other nonmetallic substrates. Particular attention is paid to developing and applying objective criteria that allow an estimation of the reliability of a particular structural determination.

337

Viscosity and Thermal Conductivity of Nitrogen for a Wide Range of Fluid States - K. Stephan, R. Krauss, and A. Laesecke. *J. Phys. Chem. Ref. Data* 16, 993 (1987).

The viscosity and the thermal conductivity of fluid nitrogen were critically evaluated and correlated on the basis of a comprehensive literature survey. Recommended values were generated in a temperature range from 70 to 1100 K and pressures up to 100 MPa using the residual concept. To retain consistency with the IUPAC Thermodynamic Tables, the same thermodynamic key data were used. Additionally, a so-called transport equation of state was established that makes it possible to achieve a unified representation of the viscosity and thermal conductivity in terms of pressure and temperature.

338

Pressure and Density Series Equations of State for Steam as Derived from the Haar-Gallagher-Kell Formulation - R. A. Dobbins, K. Mohammed, and D. A. Sullivan. *J. Phys. Chem. Ref. Data* 17, 1 (1988).

Two equations of state for the properties of steam, which are in the form of power series in pressure and density, are developed from the HGK84 formulation. These equations are of high accuracy in the equilibrium region where extensive measurements exist. They also accurately represent the extrapolated data in the metastable region between the vapor saturation and spinodal lines. The accuracy of the representations as a function of the number of terms of the series is presented.

339

Absolute Cross Sections for Molecular Photoabsorption, Partial Photoionization, and Ionic Photofragmentation Processes - J. W. Gallagher, C. E. Brion, J.A.R. Samson, and P.W. Langhoff. *J. Phys. Chem. Ref. Data* 17, 9 (1988).

A compilation is provided of absolute total photoabsorption and partial-channel photoionization cross sections for the valence shells of selected molecules, including diatomics (H_2 , N_2 , O_2 , CO , NO) and triatomics (CO_2 , N_2O), simple hydrides (H_2O , NH_3 , CH_4), hydrogen halides (HF , HCl , HBr , HI), sulfur compounds (H_2S , CS_2 , OCS , SO_2 , SF_6), and chlorine compounds (Cl_2 , CCl_4).

340

Energy Levels of Molybdenum, Mo I through Mo XLII - Jack Sugar and Arlene Musgrove. *J. Phys. Chem. Ref. Data* 17, 155 (1988).

The energy levels of the molybdenum atom, in all stages of ionization for which experimental data are available, have been compiled. Ionization energies, either experimental or theoretical, and experimental g-factors are given. Leading components of calculated eigenvectors are listed.

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups I. Benzene Series - Robert A. Alberty and Andrea K. Reif. *J. Phys. Chem. Ref. Data* 17, 241 (1988).

The polycyclic aromatic hydrocarbons can be organized into an infinite number of series in each of which successive isomer groups differ by C_4H_2 . The first series starts with benzene, and chemical thermodynamic tables are presented here for C_6H_6 , $C_{10}H_8$, $C_{14}H_{10}$, $C_{18}H_{12}$, $C_{22}H_{14}$, and $C_{26}H_{16}$ in the ideal gas phase.

342

Electronic Energy Levels of Small Polyatomic Transient Molecules - Marilyn E. Jacox. *J. Phys. Chem. Ref. Data* 17, 269 (1988).

The experimentally determined electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 6 atoms are tabulated, together with the associated vibrational structure, the radiative lifetime, the principal rotational constants, and references to the pertinent literature. Vibrational and rotational data for the ground state are also given. Observations in the gas phase, in molecular beams, and in rare-gas and nitrogen matrices are included. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and ultraviolet photoelectron spectroscopy.

343

Critical Review of Rate Constants for Reactions of Hydrated Electrons, Hydrogen Atoms and Hydroxyl Radicals ($\cdot OH/\cdot O\cdot$) in Aqueous Solution - George V. Buxton, Clive L. Greenstock, W. Phillip Helman and Alberta B. Ross. *J. Phys. Chem. Ref. Data* 17, 513 (1988).

Kinetic data for the radicals $H\cdot$ and $\cdot OH$ in aqueous solution, and the corresponding radical anions, $\cdot O^-$ and e_{aq}^- , have been critically reviewed. Reactions of the radicals in aqueous solution have been studied by pulse radiolysis, flash photolysis and other methods. Rate constants for over 3,500 reactions are tabulated, including reactions with molecules, ions and other radicals derived from inorganic and organic solutes.

344

Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane - Wing Tsang. *J. Phys. Chem. Ref. Data* 17, 887 (1988).

This publication contains evaluated and estimated data on the kinetics of reactions involving propane, isopropyl radical, n-propyl radical, and various small inorganic and organic species which are of importance for proper understanding of propane pyrolysis and combustion. It is meant to be used in conjunction with the kinetic data given in earlier publications which are of direct pertinence to the understanding of methane pyrolysis and combustion, but which also contain a large volume of data that are applicable to the propane system. The temperature range covered is 300-2500 K and the density range 1×10^{16} to 1×10^{21} molecules cm^{-3} .

345

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen $O(^3P)$ with Saturated Organic Compounds in the Gas Phase - John T. Herron. *J. Phys. Chem. Ref. Data* 17, 967 (1988).

Rate constants and mechanisms for the gas phase reactions of atomic oxygen $O(^3P)$ with organic compounds having only saturated C-C bonds are compiled and critically evaluated. Data are given for the alkanes, cycloalkanes, haloalkanes, oxygen and nitrogen containing organic compounds, and free radicals.

346

Rate Constants for Reactions of Inorganic Radicals in Aqueous Solution - P. Neta, Robert E. Huie and Alberta B. Ross. *J. Phys. Chem. Ref. Data* 17, 1027 (1988).

Rate constants have been compiled for reactions of various inorganic radicals produced by radiolysis or photolysis, as well as by other chemical means, in aqueous solutions. Data are included for the reactions of $\cdot CO_2^-$, $CO_3^{\cdot -}$, O_3 , $\cdot N_3$, $\cdot NH_2$, NO_3^{\cdot} , $\cdot PO_3^{2-}$, $PO_4^{\cdot 2-}$, $SO_2^{\cdot -}$, $\cdot SO_3^-$, $SO_4^{\cdot -}$, $SO_5^{\cdot -}$, $SeO_3^{\cdot -}$, $(SCN)_2^{\cdot -}$, $Cl_2^{\cdot -}$, $Br_2^{\cdot -}$, $I_2^{\cdot -}$, ClO_2^{\cdot} , BrO_2^{\cdot} , and miscellaneous related radicals, with inorganic and organic compounds.

347

Recommended Data on the Electron Impact Ionization of Atoms and Ions: Fluorine to Nickel - M. A. Lennon, K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, M. J. Murray, and F. J. Smith. *J. Phys. Chem. Ref. Data* 17, 1285 (1988).

Experimental and theoretical cross-section data for electron impact ionization of atoms and ions from fluorine to nickel has been assessed and earlier recommendations for light atoms and ions have been revised. Based on this assessment and, in the absence of any data, on the classical scaling laws, a recommended cross section has been produced for each species.

348

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen $O(^3P)$ with Sulfur Containing Compounds - D. L. Singleton and R. J. Cvetanovic. *J. Phys. Chem. Ref. Data* 17, 1377 (1988).

Chemical kinetic data for reactions of $O(^3P)$ atoms with sulfur containing compounds are compiled and critically evaluated. Specifically, the reactions considered include the interactions of the ground electronic state of oxygen atoms, $O(^3P)$, with S_2 , SF_2 , SF_5 , SOF , S_2O , SO , SO_2 , SO_3 , SH , H_2S , D_2S , H_2SO_4 , CS , CS_2 , COS , CH_3SH , C_2H_5SH , C_3H_7SH , C_4H_9SH , $C_5H_{11}SH$, CH_3SCH_3 , $cy-CH_2SCH_2$, $cy-CHCH-SCHCH$, CH_3SSCH_3 , SCF_3 , $SCCl_2$, and $cy-CF_2SCF_2S$. With one exception, the liquid phase reaction $O(^3P) + H_2SO_4 \rightarrow$ products, all the data considered were for gas phase reactions.

349

New International Skeleton Tables for the Thermodynamic Properties of Ordinary Water Substance H. Sato, M. Uematsu, K. Watanabe, A. Saul, and W. Wagner. *J. Phys. Chem. Ref. Data* 17, 1439 (1988).

The current knowledge of thermodynamic properties of ordinary water substance is summarized in a condensed form of a set of skeleton steam tables, where the most probable values with the reliabilities on specific volume and enthalpy are provided in the range of temperatures from 273 to 1073 K and pressures from 101.235 kPa to 1 GPa and at the saturation state from the triple point to the critical point. These tables have been accepted as the IAPS Skeleton Tables 1985 for the Thermodynamic Properties of Ordinary Water Substance (IST-85) by the International Association for the Properties of Steam (IAPS).

350

Benzene Thermophysical Properties from 279 to 900 K at Pressures to 1000 Bar - Robert D. Goodwin. *J. Phys. Chem. Ref. Data* 17, 1541 (1988).

The thermodynamic data for benzene have been evaluated and fit to a highly constrained, nonanalytic equation of state. Comparisons of the equation with the selected PVT and derived property data are given. Extensive tables are presented providing tabular values for co-existing liquid and vapor as well as for the single phase along isobars. The equation of state and tables cover the range from the triple point (278.68 K) to 900 K, with pressures to 1000 bar.

351

Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15 K - Eugene S. Domalski and Elizabeth D. Hearing. *J. Phys. Chem. Ref. Data* 17, 1637 (1988).

An estimation method developed by S. W. Benson and coworkers, for calculating the thermodynamic properties of organic compounds in the gas phase, has been extended to the liquid and solid phases for hydrocarbon compounds at 298.15 K.

Wavelengths and Energy Level Classifications of Scandium Spectra for All Stages of Ionization - V. Kaufman and J. Sugar. *J. Phys. Chem. Ref. Data* 17, 1679 (1988).

Wavelengths and their classifications are compiled for the spectra of scandium, Sc I through Sc XXI. Selections of data are based on the critical evaluations in the compilation of energy levels by Sugar and Corliss. These are updated by a thorough search of the subsequent literature. All classifications are verified with predictions made by differencing the energy levels. Spectra are ordered by ionization stage and listed by wavelength. Two finding lists are included, one containing Sc I to Sc III and the other Sc IV to Sc XXI.

353

Atomic Weights of the Elements 1987 - J. R. De Laeter. *J. Phys. Chem. Ref. Data* 17, 1791 (1988).

The International Union of Pure and Applied Chemistry Commission on Atomic Weights and Isotopic Abundances has reviewed recent literature and confirmed the atomic weight values published in 1985, with one minor change. The current table of standard atomic weights is presented.

354

The 1986 CODATA Recommended Values of the Fundamental Physical Constants - E. Richard Cohen and Barry N. Taylor. *J. Phys. Chem. Ref. Data* 17, 1795 (1988).

Presented here are the values of the basic constants and conversion factors of physics and chemistry resulting from the 1986 least-squares adjustment of the fundamental physical constants as published by the CODATA (Committee on Data for Science and Technology) Task Group on Fundamental Constants and recommended for international use by CODATA. The 1986 CODATA set of values replaces its predecessor published by the Task Group and recommended for international use by CODATA in 1973.

355

Standard Electrode Potentials and Temperature Coefficients in Water at 298.15 K - Steven G. Bratsch. *J. Phys. Chem. Ref. Data* 18, 1 (1989).

A great deal of solution chemistry can be summarized in a table of standard electrode potentials of the elements in the solvent of interest. In this work, standard electrode potentials and temperature coefficients in water at 298.15 K, based primarily on the "NBS Tables of Chemical Thermodynamic Properties," are given for nearly 1700 half-reactions at pH = 0.000 and pH = 13.996. The data allow the calculation of the thermodynamic changes and equilibrium constants associated with ~1.4 million complete cell reactions over the normal temperature range of liquid water.

356

Cross Sections for Collisions of Electrons and Photons with Oxygen Molecules - Y. Itikawa, A. Ichimura, K. Onda, K. Sakimoto, K. Takayanagi, Y. Hatano, M. Hayashi, H. Nishimura, and S. Tsurubuchi. *J. Phys. Chem. Ref. Data* 18, 23 (1989).

Data have been compiled on the cross sections for collisions of electrons and photons with oxygen molecules (O_2). For electron collisions, the processes included are: total scattering, elastic scattering, momentum transfer, excitations of rotational, vibrational, and electronic states, dissociation, ionization, and attachment. Ionization and dissociation processes are considered for photon impact.

357

Thermal Conductivity of Refrigerants in a Wide Range of Temperature and Pressure - R. Krauss and K. Stephan. *J. Phys. Chem. Ref. Data* 18, 43 (1989).

Thermal conductivities of refrigerant 12 (dichlorodifluoromethane), refrigerant 113 (1,1,2-trichloro-1,2,2-trifluoroethane), refrigerant 114 (1,2-dichloro-1,1,2,2-tetrafluoroethane), and refrigerant C318 (perfluorocyclobutane) were critically evaluated and correlated on the basis of a comprehensive literature survey. Recommended values were established for a wide range of temperatures and pressures, extending up to three times the critical density and excluding the critical region.

358

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. II. Pyrene Series, Naphthopyrene Series, and Coronene Series - Robert A. Alberty, Michael B. Chung, and Andrea K. Reif. *J. Phys. Chem. Ref. Data* 18, 77 (1989).

The tables in the first paper on polycyclic aromatic hydrocarbons [*J. Phys. Chem. Ref. Data* 17, 241 (1988)] have been extended by calculating thermodynamic properties for the first four isomer groups in the pyrene series, the first three isomer groups in the naphthopyrene series, and the first three isomer groups in the coronene series.

359

Cross Sections for K-Shell X-Ray Production by Hydrogen and Helium Ions in Elements from Beryllium to Uranium - G. Lapicki. *J. Phys. Chem. Ref. Data* 18, 111 (1989).

Experimental cross sections for K-shell x-ray production by hydrogen and helium ions ($Z_1 = 1, 2$) in target atoms for beryllium to uranium ($Z^2 = 4-92$) are tabulated as compiled (7418 cross sections) from the literature (161 references were found) with the search for the data terminated in January 1988.

360

Rate Constants for the Quenching of Excited States of Metal Complexes in Fluid Solution - Morton Z. Hoffman, Fabrizio Bolletta, Luca Moggi, and Gordon L. Hug. *J. Phys. Chem. Ref. Data* 18, 219 (1989).

The rate constants for the quenching of the excited states of metal ions and complexes in homogeneous fluid solution are reported in this compilation. Values of K_q for dynamic, collisional processes between excited species and quenchers have been critically evaluated, and are presented with the following information, among others, from the original publications, when available: description of the solution medium, temperature at which K_q was determined, experimental method, range of quencher concentration used, lifetime of the excited state in the absence of quencher, activation parameters, quenching mechanism.

361

The Thermal Conductivity of Nitrogen and Carbon Monoxide in the Limit of Zero Density - J. Millat and W. A. Wakeham. *J. Phys. Chem. Ref. Data* 18, 565 (1989).

The paper presents accurate representations for the thermal conductivity of the diatomic gases nitrogen and carbon monoxide in the limit of zero density. These gases were studied because they have nearly the same molecular mass and viscosities. In contrast, the new analysis confirms that the thermal conductivities of the two gases differ remarkably, especially at low temperatures.

362

Thermophysical Properties of Methane - Daniel G. Friend, James F. Ely and Hepburn Ingham. *J. Phys. Chem. Ref. Data* 18, 583 (1989).

New correlations for the thermophysical properties of fluid methane are presented. The correlations are based on a critical evaluation of the available experimental data and have been developed to represent these data over a broad range of the state variables. Estimates for the accuracy of the equations and comparisons with measured properties are given. The reasons for this new study of methane include significant new and more accurate data, and improvements in the correlation functions which allow increased accuracy of the correlations, especially in the extended critical region.

Thermodynamic Properties of Argon from the Triple Point to 1200 K with Pressures to 1000 MPa - Richard B. Stewart and Richard T. Jacobson. *J. Phys. Chem. Ref. Data* 18, 639 (1989).

A new thermodynamic property formulation for argon is presented. The formulation includes a fundamental equation explicit in Helmholtz energy, a vapor pressure equation, and estimating functions for the densities of saturated liquid and vapor states.

364

Thermodynamic Properties of Dioxygen Difluoride (O_2F_2) and Dioxygen Fluoride (O_2F) - John L. Lyman. *J. Phys. Chem. Ref. Data* 18, 799 (1989).

Recent spectroscopic and chemical kinetic studies have provided sufficient data for construction of reliable thermodynamic tables for both dioxygen difluoride (O_2F_2 ; Chemical Abstracts Registry Number, 7783-44-0) and oxygen fluoride (O_2F ; Chemical Abstracts Registry Number, 15499-23-7). This paper contains those tables for these species in both SI units (0.1 MPa standard state) and cal-K-mol units (1.0 atm standard state).

365

Thermodynamic and Transport Properties of Carbohydrates and their Monophosphates: The Pentoses and Hexoses - Robert N. Goldberg and Yadu B. Tewari. *J. Phys. Chem. Ref. Data* 18, 809 (1989).

This review contains recommended values of the thermodynamic and transport properties of the five and six membered ring carbohydrates and their phosphates in both the condensed and aqueous phases. Equilibrium data, enthalpies, heat capacities, and entropies have been collected from the literature.

366

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supplement III - R. Atkinson, D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr and J. Troe. *J. Phys. Chem. Ref. Data* 18, 881 (1989).

This paper updates and extends previous critical evaluations of the kinetics and photo-chemistry of gas phase chemical reactions of neutral species involved in atmosphere chemistry [*J. Phys. Chem. Ref. Data* 19, 295 (1980); 11, 327 (1982); 13, 1259 (1984)]. The work has been carried out by the authors under the auspices of the IUPAC Subcommittee on Gas Phase Kinetic Data Evaluation for Atmospheric Chemistry.

367

Octanol-Water Partition Coefficients of Simple Organic Compounds - James Sangster. *J. Phys. Chem. Ref. Data* 18, (1989).

Octanol-water partition coefficients (Log P) for 611 simple organic compounds have been retrieved from the literature. All principal classes of compounds are represented. Available experimental details of measurement have also been retrieved from original articles. Pertinent thermodynamic relations are presented in some detail, together with a discussion of direct and indirect methods of measurement. Reported Log P data for each compound have been evaluated according to state criteria, and recommended values (with uncertainty) are given as a guide to users.

368

Solubility of Simple Apolar Gases in Light and Heavy Water at High Temperature: A Critical Assessment of Data - Roberto Fernandez Prini and Rosa Crovetto. *J. Phys. Chem. Ref. Data* 18, (1989).

The systems that have been included in this work are the inert gases and CH_4 in light water and heavy water, H_2 , O_2 , N_2 and C_2H_6 in light

water and D_2 in heavy water. Data reported in the original sources have been brought to the same footing by back calculating the raw experimental data, a step considered necessary to assess critically the available sets of data. The temperature dependence of Henry's constants for all the binary systems have been expressed in terms of two polynomial equations. The formulations presented here are discussed and the limits of application given.

369

Microwave Spectral Tables III. Hydrocarbons, CH to $C_{10}H_{10}$ - F. J. Lovas and R. D. Suenram. *J. Phys. Chem. Ref. Data* 18, (1989).

All of the rotational spectral lines observed and reported in the open literature for 91 hydrocarbon molecules have been tabulated. The isotopic molecular species, assigned quantum numbers, observed frequency, estimated measurement uncertainty and reference are given for each transition reported. The derived molecular properties, such as rotational and centrifugal distortion constants, hyperfine structure constants, electric dipole moments, and rotational g-factors are listed.

370

A Fundamental Equation for Water Covering the Range from the Melting Line to 1273 K at Pressures up to 25000 MPa - A. Saul and W. Wagner. *J. Phys. Chem. Ref. Data* 18, (1989).

In order to represent the thermodynamic properties of water (H_2O) over an extremely large range of temperature and pressure that is not covered by existing equations of state, a new fundamental equation has been developed.

371

Toluene Thermophysical Properties from 178 to 800 K at Pressures to 1000 Bar - Robert D. Goodwin. *J. Phys. Chem. Ref. Data* 18, (1989).

The thermodynamic data for toluene have been evaluated and fit to a highly-constrained, nonanalytic equation of state. Comparisons of the equation with the selected PVT and derived property data are given. Extensive tables are presented providing tabular values for co-existing liquid and vapor as well as for the single phase along isobars. The equation of state and tables cover the range from the triplet point (178.15 K) to 800 K, with pressures to 1000 bar.

372

Reduction Potentials of One-electron Couples Involving Free Radicals in Aqueous Solution - Peter Wardman. *J. Phys. Chem. Ref. Data* 18, (1989).

Tables of 1200 values of reduction potentials of 700 one-electron couples in aqueous solution are presented. The majority of organic oxidants listed are quinones, nitroaryl and bipyridinium compounds. Reductants include phenols, aromatic amines, indoles and pyrimidines, thiols and phenothiazines. Inorganic couples largely involve compounds of oxygen, sulfur nitrogen and the halogens.

373

Photoemission Cross Sections for Atomic Transitions in the Extreme Ultraviolet due to Electron Collisions with Atoms and Molecules - P. J. M. van der Burgt, W. B. Westerveld and J. S. Risley. *J. Phys. Chem. Ref. Data* 18, (1989).

This article reviews experimental photoemission cross sections in the extreme ultraviolet, for transitions in excited atoms and atomic ions formed in electron collisions with atoms and molecules. A survey of the available experimental data for each investigated target gas reveals severe inconsistencies between cross sections reported by different laboratories. As almost all reported cross sections are based on relative measurements, a detailed discussion is given of the methods used for normalization of the cross sections.

Supplements

Atomic and Ionic Spectrum Lines below 2000 Angstroms: Hydrogen Through Krypton-Raymond L. Kelly. *J. Phys. Chem. Ref. Data* 16, Suppl. 1 (1987).

With over 1600 pages of evaluated data, this compilation provides a comprehensive reference source for vacuum ultraviolet spectra of the first 36 elements. In addition to wavelength and intensity, the upper and lower energy levels, configurations, and terms are presented for each line. References are given to the sources of all data.

Gas-Phase Ion and Neutral Thermochemistry-S. G. Lias, J. E. Bartmess, J. L. Holmes, R. D. Levin, J. F. Liebman, and W. G. Mallard. *J. Phys. Chem. Ref. Data* 17, Suppl. 1 (1988).

This volume includes evaluated ionization energies of 4000 atoms and molecules and proton affinities of 1000 compounds, as well as electron affinities and gas phase acidities of approximately 3000 species. The thermochemistry of the related neutral species is also given.

Thermodynamic and Transport Properties for Molten Salts: Correlation Equations for Critically Evaluated Density, Surface Tension, Electrical Conductance and Viscosity Data-G. J. Janz. *J. Phys. Chem. Ref. Data* 17, Suppl. 2 (1988).

The best-value recommendations previously advanced have been re-examined, upgraded, and consolidated in this important data source, together with additions from the open scientific literature through 1987 and early 1988. For each system, the recommended values are reported

in the form of equations, together with uncertainty statements, and references to the detailed evaluations.

Atomic Transition Probabilities, Scandium Through Manganese-G. A. Martin, J. R. Fuhr, and W. L. Wiese. *J. Phys. Chem. Ref. Data* 17, Suppl. 3 (1988).

Atomic Transition Probabilities, Iron Through Nickel-J. R. Fuhr, G. A. Martin and W. L. Wiese. *J. Phys. Chem. Ref. Data* 17, Suppl. 4 (1988).

These two supplements contain almost 18,000 atomic transition probabilities. The data are presented by element and spectrum. To facilitate locating the transitions, finding lists ordered by wavelength are provided at the beginning of each spectrum. In addition to the spectroscopic classifications, the wavelengths of the transitions, the lower and upper energy level values and their statistical weights are given.

Monographs

Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds - Roger Atkinson. *J. Phys. Chem. Ref. Data Monograph* 1, (1989).

The literature kinetic and mechanistic data for the gas-phase reactions of the OH radical with organic compounds (through 1988) have been tabulated, reviewed and evaluated over the entire temperature ranges for which data are available.

Standard Reference Databases

NIST/EPA/MSDC Mass Spectral Database

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The NIST/EPA/MSDC Mass Spectral Database has been assembled from a variety of sources in a joint program of the Environmental Protection Agency, The National Institutes of Health, the United Kingdom Mass Spectrometry Data Center and the National Institute of Standards and Technology.

The database contains ionization mass spectra of 50,000 different compounds. Each spectrum has a "quality index" associated with it, the Chemical Abstracts Service (CAS) name, synonyms, the molecular weight and formula and the CAS registry number. Structures have recently been included for 85% of the spectra. Categories of substances identified are steroids, alkaloids, drugs, derivatives, amino acids, metals, carbohydrates, fatty acids and lipids, pesticides and primary pollutants.

This database is available as a magnetic tape, both in ASCII and standard IBM unformatted FORTRAN G. It is also available online through STN and CIS and internationally.

NIST/EPA/MSDC Mass Spectral Database PC Version 2.0

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The PC Version of this database was released in September 1987. Version 2.0 was released in December 1988. The PC Version consists of the database of 50,000 electron ionization mass spectra, various index files for rapid data retrieval and related software for searching the database in various ways. The database can be searched by:

- identification number
- CAS Registry number
- chemical name
- molecular formula-can also specify up to 10 peaks
- molecular weight-can also specify partial elemental composition up to 10 peaks
- major peaks
 - more than one set of ordered peaks
 - molecular weight
 - elements in the unknown
 - all elements possibly in the unknown
 - numbers of atoms of each element
 - up to 10 peaks with abundance ranges

Version 2.0 has many new searching features.

- complete sequential search and re-search of the entire database
- individual peaks
- automatic searching
- command line options

Another new feature is the utility to add the user's own spectra to the database.

The PC Version of this database is available in AT and PSII versions.

NIST Chemical Thermodynamics Database

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This database contains recommended values for selected thermodynamic properties for more than 15,000 inorganic substances. These properties include the following:

- 1) Standard state properties at 298.15 K and 1 bar
 - enthalpy of formation from the elements in their standard state
 - Gibbs (free) energy of formation from the elements in their standard state
 - entropy
 - enthalpy $H^\circ(298.15 \text{ K}) - H^\circ(0 \text{ K})$
 - heat capacity at constant pressure
- 2) At 0 K
 - enthalpy of formation

The database is not presently supplied with search software, but a PC Version is currently in preparation. It is available in a magnetic tape format and online through STN and CIS.

NIST Crystal Data Identification File

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This file contains crystallographic information useful to characterize more than 60,000 inorganic and organic crystalline materials. The data include the reduced cell parameters, reduced cell volume, space group number and symbol, the calculated density, classification by chemical type, chemical formula and chemical name. Each entry has an associated literature reference.

The database can be utilized as a practical analytical tool for compound characterization and identification because the reduced cell (i.e., the lattice) is unique for most compounds. Unknowns can be conveniently identified by the following sequence:

- 1) determine a primitive or centered cell for an unknown to a crystal;
- 2) calculate the reduced cell; and
- 3) search for a match with an entry in the NIST Crystal Data Identification File.

The database can also be utilized to prevent redeterminations of published structures. It is also useful in conjunction with other data for materials characterization.

The file includes reliable data across the entire spectrum of the solid state including inorganics, organics, minerals intermetallics, metals, alloys, drugs, antibiotics, and pesticides. Search software, NBS*LATTICE, is also provided with the database. The search software provides symmetry and pseudosymmetry determinations, subcell and supercell calculations done systematically, cell transformations, matrix inversions, and identification via lattice matching.

This database is available in magnetic tape and CD ROM formats and is available internationally online. Please contact JCPDS-International Centre for Diffraction Data, 1661 Park Lane, Swarthmore, PA 19081.

NIST Thermophysical Properties of Hydrocarbon Mixtures

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This database (called TRAPP) allows the interactive prediction of thermophysical properties of hydrocarbon mixtures. The properties calculated include density, viscosity, and thermal conductivity. The model used is valid over a wide range of pressure and temperature conditions and covers hydrocarbons up to C_{20} , plus several other common fluids. The method of calculation is applicable to a wide variety of chemical types, to thermodynamic states ranging from the dilute gas to compressed liquid, and to multicomponent systems.

The model used has been extensively compared with experimental data for pure fluids and binary mixtures. The average percentage deviation for both viscosity and thermal conductivity was observed to be less than 8%.

Upon execution, the program will ask the user:

- 1) if he wishes to see a list of chemical components;
- 2) if he desires metric or engineering units;
- 3) number of components present in the mixture;
- 4) number of moles of each component;
- 5) temperature and pressure at which properties are to be calculated; and
- 6) if the user desires a vapor calculation.

Finally, the software allows a recalculation with specific changes in parameters.

This database is available in a magnetic tape version. A new SUPER TRAPP is planned for the future.

NIST Electron and Positron Stopping Powers of Materials

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This database (called EPSTAR) contains data related to the electron and positron stopping powers of various materials. Included in EPSTAR are collision, radiative, and total stopping powers; ranges, radiation yields and auxiliary information (density-effect correction, coefficients of variation of collision stopping power, range and

bremsstrahlung yield with respect to the mean excitation of the medium). Data are included for electrons in 285 materials for positrons in 29 materials, at energies from 10 keV to 10 GeV.

EPSTAR is an interactive program; the user can select to see a listing of the materials for which the data are available and choose the material for which the data are to be presented as well as the energy range over which those data are desired.

This database is available in a magnetic tape format. A new PC version is planned for the near future.

NIST X-Ray and Gamma-Ray Cross Section and Attenuation Coefficients

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This database (called XGAM) provides photon cross sections (interaction coefficients) and attenuation coefficients for any substance. Interactive software is provided which enables the user to obtain data by entering chemical formulas or other measures of composition for a mixture of component materials. The user may also select the energy range over which data are desired.

The system operates from a database of cross sections for coherent and incoherent scattering, photoionization and pair production for the elements $Z = 1$ to 100 at energies from 1 keV to 100 GeV. The data supplied were obtained by a critical data analysis combining theoretical and experimental results.

The user may request data to be tabulated at the fixed energies stored in the database, at these fixed energies plus others specified by the user, or at completely arbitrary set of specified energies. The tabulated results include the individual contributions and the total mass attenuation coefficient, with and without coherent scattering.

This database is available on both a PC diskette and a magnetic tape.

NIST Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions

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This database (called GAMPHI) provides values of activity and osmotic coefficients of binary aqueous electrolyte solutions at 298.15 K together with a collection of subroutines for utilizing this database. These thermodynamic properties are needed when performing equilibrium calculations on aqueous solutions.

Each binary electrolyte solution contains the name of the cation and anion in the binary salt; the literature reference from which the data were obtained; the minimum and maximum molality for which the data are valid; a designation of an internal database name to which the data set belongs; a designation as to whether or not the data are considered to be primary or nonprimary for a given salt in the entire database; an integer which indicates which equation or model is used to calculate the value of activity and osmotic coefficients; the number of parameters in the model and the parameters of the model.

This database is available in magnetic tape format.

NIST Thermophysical Properties of Water

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This database consists of an interactive program which calculates the thermodynamic properties of fluid H_2O (liquid and vapor) using the formulation as approved by the International Association for the Properties of Steam (IAPS) at its Tenth International Conference in 1984.

The interactive FORTRAN 77 program consists of three parts. The first part contains a package of subroutines to calculate the thermodynamic and transport properties of fluid H_2O . The remaining two call these routines to generate properties of H_2O interactively.

The first main program allows the calculation and display of all properties at a single pair of independent variables:

pressure - temperature
density - temperature
entropy - temperature
enthalpy - temperature
enthalpy - pressure

The second main program allows the generation of tables of properties along isotherms, isobars, or isochores. To keep the tabular form compact, the user may choose which properties are to be displayed.

The range approved by IAPS for this formulation includes temperatures from 0 to 1000° C with pressures up to 1500 MPa and down to 0 MPa. The range over which usable results will be obtained extends to 2250° and to 3000 MPa.

The printed version of this database, which includes a description of the data selection and evaluation procedures, is found in L. Haar, J.S. Gallagher, and G.S. Kell, "NBS/NRC Steam Tables", Hemisphere Press, Washington, DC, 1984. This database is available in both tape and diskette version.

DIPPR Data Compilation of Pure Compound Properties

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The DIPPR database contains data on 39 properties for 1023 chemical compounds. These data were released for public distribution by the Design Institute for Physical Property Data (DIPPR) in November 1984. Thermodynamic, physical, transport and environmental property data are given for pure chemical compounds of high industrial priority. The database was prepared by Pennsylvania State University for the Design Institute for Physical Property Data, a cooperative project sponsored by 50 major chemical manufacturers and related companies under the auspices of the American Institute of Chemical Engineers.

For each chemical compound included, values are given for 26 single-valued property constants and for 13 properties as functions of temperature, calculated for correlation coefficients. The database also

includes estimates of the accuracy of each property value and references to the sources of measured or predicted data which were used in selecting the recommended values. The database includes numeric values, as well as interactive software which allows access to specific properties of the compounds included, in any specified set of units.

This database is available in magnetic tape and diskette format.

NIST Thermophysical Properties of Fluids

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These interactive programs (called MIPROPS) compute thermophysical properties of twelve pure fluids: helium, argon, parahydrogen, oxygen, nitrogen, nitrogen trifluoride, ethylene, methane, ethane, propane, isobutane, and normal butane. The programs provide prompting for selection of several options including choice of fluid; choice of SI or engineering units and choice of single phase or liquid vapor phase calculations.

Properties are computed for the single phase region from input of two of the following variables: temperature, pressure, and density. Values on the liquid-vapor boundary are computed for either a given temperature or a given pressure. The program returns values for pressure, temperature, density, internal energy, enthalpy, entropy, specific heats at constant volume and pressure and sound velocity. Viscosity, thermal conductivity and dielectric constant are given for five of the fluids.

This database is available in PC diskette and magnetic tape format.

NIST JANAF Thermochemical Tables

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The JANAF Thermochemical Tables provide a compilation of critically evaluated thermodynamic properties of approximately 1800 substances over a wide range of temperature. Recommended temperature-dependent values are provided for chemical thermodynamic properties of inorganic substances and for organic substances containing only one or two carbon atoms.

These tables cover the thermodynamic properties with single phase and multiphase tables for the crystal, liquid, and ideal gas state. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states. All values are given in SI units and are for a standard state pressure of 100,000 pascal (1 bar). Each tabulation is the result of a critical evaluation of the literature upon which the thermochemical table is based.

At present, this database is available on magnetic tape. A new PC version of this database is currently in preparation.

NIST Mixture Property Program

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The NIST Mixture Property Program (DDMX) is an interactive computer program which calculates various thermodynamic and transport properties of mixtures of fluids selected from any of seventeen possible pure components. The emphasis of the program is on density prediction (especially for CO₂ rich mixtures) but it will provide accurate results for other properties and mixtures.

All phase equilibrium calculations are performed with the Peng-Robinson (PR) equation of state, and co-existing phase properties are calculated with the NIST extended corresponding states model (DDMX). Mixtures formed from any of seventeen pure components (including hydrocarbons, N₂, O₂, Ar, CO, CO₂ and H₂S) are handled by the program.

DDMX provides the following outputs for any specified mixture:

- bubble point pressure;
- dew point pressure;
- saturation properties;
- tables of density, enthalpy, entropy, and heat capacity as a function of T or P; and
- isothermal flash calculation yielding density, enthalpy, entropy, heat capacity, viscosity and thermal conductivity of feed and vapor.

This database is available in PC diskette format.

NIST/Sandia/ICDD Electron Diffraction Database

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This database is designed for phase characterization obtained by electron, neutron or x-ray diffraction methods. The database and associated software permit highly selective identification procedures for microscopic, as well as macroscopic crystalline materials. The database contains chemical, physical and crystallographic information on a wide variety of materials including minerals, metals, intermetallics and general inorganic compounds. The Electron Diffraction Database has been designed to include all the data required to identify materials using computerized d-spacing/formula matching techniques. The data for each entry include the conventional cell, reduced cell, lattice type, space group, calculated or observed d-spacings, chemical name, chemical and empirical formula, material class indicators, references and other parameters.

This database is available in magnetic tape format.

NIST Corrosion Performance Database

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These are two PC databases on the corrosion performance of metals and non-metallics. Cor-Sur Volume 1 has data for 25 metallic materials exposed to about 1000 corrosive environments at various temperatures and concentrations. Cor-Sur Volume 2 has similar data for 36 elastomers, polymers and composites. Retrieved data can be displayed in tables and graphs. The data are derived from NACE Corrosion Data Surveys and are products of the NACE-NIST corrosion Data Program.

NIST Chemical Kinetics Database

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The NIST Chemical Kinetics Database is designed to provide rapid access to kinetics data for gas phase reactions including surveys of the literature on a particular reaction, all of the reactions of a given species, subsets of all of the reactions and the data available from a given paper. A highly interactive program allows users to search by reactants or by reference. The database contains more than 2000 separate reactions and 6600 records. The results of a search can be graphically displayed and mathematically fit to standard kinetic equations.

The database contains the following information on each rate constant record:

- Reactants and, if defined, products of the reaction;
- Rate parameters: A, n, (E_a/R) where $k = A (T/298)^n \exp(-E_a/R/T)$;
- Uncertainty in A, n, and E_a/R if reported;
- Temperature range of experiment, or temperature range of validity for a review or theoretical paper;
- Pressure range and bulk gas of the experiment;
- Data type of the record; i.e. direct measurement, relative rate measurement, theoretical, etc.; and
- Experimental procedure, including analytical procedures, excitation technique, etc.

This database is available in PC diskette format.

NSRDS-NIST Series

73 Part 1

Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971-1982)-Francis Westley, John T. Herron, and R. J. Cvetanovic. NSRDS-NBS 73, Part 1, 673 p. (1987).

Chemical kinetics data for reactions of importance in combustion chemistry are compiled. Data are given for 1931 reactions.

73 Part 2

Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 2. Non-Aromatic C, H, O, N, and S Containing Compounds. (1983)-Francis Westley, John T. Herron, and R. J. Cvetanovic. NSRDS-NBS 73, Part 2, 135 p. (1987).

Chemical kinetics data for reactions of importance in combustion chemistry are compiled. Data were taken from the literature published in 1983. Data omitted from Part 1 of this series, covering the period 1971 to 1982 are also included. Data are given for 434 reactions.

NIST Technical Notes

1249

Evaluation of Data Availability and Quality for Interaction Second Virial Coefficients of Use to the Gas Industry.-Bernard J. Van Wie, Mark A. Langenberg, Wayne C.-W. Chang, Kesavalu H. Kumar, and Kenneth E. Starling. NBS Tech. Note 1249, 90 p. (1988).

Binary interaction second virial coefficient information useful to the natural and syngas industries has been compiled and evaluated. An extensive literature search has been conducted to obtain publicly available information dating back to 1900. Each binary gas system has been individually evaluated and references containing the highest quality and most abundant measurements have been listed in a table of recommended values.

1325

Tables for the Thermophysical Properties of Methane-Daniel G. Friend, James F. Ely, and Hepburn Ingam. NIST Technical Note 1325, 478 p. (1989).

The thermophysical properties of methane are tabulated for a large range of fluid states based on recently formulated correlations. For the thermodynamic properties, temperatures from 91 to 600 K at pressures less than 100 MPa are included. For the viscosity, the corresponding range is 91-400 K with pressures to 55 MPa, while for the thermal conductivity the range is 91-600 K with pressures to 100 MPa.

NIST Special Publications

737

Towards a Tribology Information System. John Rumble, Jr. and Lewis Sibley. NBS Spec. Publ. 737, 131 p. (1987).

This report summarizes the findings of a planning workshop at the National Bureau of Standards during July and August 1985 to address the needs for a computerized tribology information and data system, as well as possible implementation schemes.

742

Computerization of Welding Information-A Workshop Report-T. A. Siewert and J. E. Jones (editors). NBS Spec. Publ. 742, 31 p. (1988).

The Workshop on Computerization of Welding Data was sponsored by the National Bureau of Standards and the American Welding

Institute to determine whether national welding productivity could be improved through the development of welding databases. The workshop grew out of the realization that this goal is now feasible since smaller, more powerful computers have become available and affordable.

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Measurements of electron impact optical excitation functions-D. W. O. Heddle and Jean W. Gallagher. Rev. Mod. Phys. 61, 221 (1989).

A Simplified Representation for the Thermal Conductivity of Fluids in the Critical Region-G. A. Olchowy and J. V. Sengers. Int. J. Thermophys. 10, 417 (1989).

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Heat Capacity of Aqueous $MgCl_2$ from 349 to 598 K-Dorothy E. White, Jeffrey A. Gates, David M. Tillet, and Robert H. Wood. J. Chem. Eng. Data 33, 485 (1988).

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Pre-exponential Temperature Dependences of Bimolecular Reaction Rate Coefficients Predicted by Transition State Theory-N. Cohen. Aerospace Report ATR-88(7073)-1 (1988).

Revised Group Additivity Values of Enthalpies for Linear Alkanes and Alkyl Radicals-N. Cohen. Aerospace Report ATR-88(7073)-2 (1988).

Thermodynamic Properties of Methane in the Critical Region-D. S. Kurumov, G. A. Olchowy, and J. V. Sengers. Int. J. of Thermophysics 9, 73 (1988).

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Vibrational spectra (infrared, Raman)

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See: Elastic constants

Ordering Information

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